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     (FILE 'HOME' ENTERED AT 08:46:14 ON 03 MAR 2005)
     FILE 'REGISTRY' ENTERED AT 08:46:44 ON 03 MAR 2005
L1
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              0 S L1
L2
              2 S L1 FUL
L3
                STRUCTURE UPLOADED
L4
L5
              0 S L4
             12 S L4 FUL
L6
     FILE 'REGISTRY' ENTERED AT 08:52:19 ON 03 MAR 2005
L7
              0 S L6
     FILE 'CAPLUS' ENTERED AT 08:52:28 ON 03 MAR 2005
              7 S L6
L8
=> d 14
L4 HAS NO ANSWERS
L4
                STR
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
Structure attributes must be viewed using STN Express query preparation.
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=> d bib abs hitstr 1-7

ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:1070486 CAPLUS

DN 142:168979

- ΤI 4-(2-[2-(2(R)-Methylpyrrolidin-1-yl)ethyl]benzofuran-5-yl)benzonitrile and Related 2-Aminoethylbenzofuran H3 Receptor Antagonists Potently Enhance Cognition and Attention
- ΑU Cowart, Marlon; Faghih, Ramin; Curtis, Michael P.; Gfesser, Gregory A.; Bennani, Youssef L.; Black, Lawrence A.; Pan, Liping; Marsh, Kennan C.; Sullivan, James P.; Esbenshade, Timothy A.; Fox, Gerard B.; Hancock, Arthur A.
- CS Department of Neuroscience Research and Department of Drug Metabolism and Pharmacokinetics, Abbott Laboratories, Abbott Park, IL, 60064-6123, USA
- SO Journal of Medicinal Chemistry (2005), 48(1), 38-55 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DTJournal
- LΑ English
- AB H3 receptor antagonists based on a 2-aminoethylbenzofuran skeleton have been discovered, which are potent in vitro at human and rat H3 receptors, with Ki values of 0.1-5.8 nM. Analogs were discovered with potent (0.01-1 mg/kg) cognition and attention enhancing properties in animal models. One compound in particular, 4-(2-[2-(2(R)-methylpyrrolidin-1-yl)ethyl]benzofuran-5-yl)benzonitrile (ABT-239), combined potent and selective H3 receptor antagonism and excellent pharmacokinetic and metabolic properties across species, with full efficacy in two behavioral models: a five-trial inhibitory avoidance acquisition model in rat pups at 0.1 mg/kg and a social recognition memory model in adult rats at 0.01 mg/kg. Furthermore, this compound did not stimulate locomotor activity and showed high selectivity for the induction of behavioral efficacy vs. central nervous system based side effects. The potency and selectivity of this compound and of analogs from this class support the potential of H3 receptor antagonists for the treatment of cognitive dysfunction.

IT 460748-54-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(4-(2-[2-(2(R)-methylpyrrolidin-1-yl)ethyl]benzofuran-5-yl)benzonitrile and related 2-aminoethylbenzofuran H3 receptor antagonists potently enhance cognition and attention)

RN 460748-54-3 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 4'-hydroxy-3'-iodo-, ethyl ester (9CI) (CA INDEX NAME)

RE.CNT 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:736244 CAPLUS

DN 137:247602

TI Preparation of (pyrrolidinylalkyl)benzofurans and analogs as histamine-3 receptor ligands for treatment of disorders related to CNS neurotransmission

IN Cowart, Marlon D.; Bennani, Youssef L.; Faghih, Ramin; Gfesser, Gregory A.; Black, Lawrence A.

PA Abbott Laboratories, USA

SO PCT Int. Appl., 268 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

GI

PAN.	PATENT NO.				KIND DATE		APPLICATION NO.			DATE									
ΡI		NO 2002074758 NO 2002074758			A2	20020926		WO 2002-US7107			20020311								
		W:	AE, CO, GM, LS, PL, UA, GH,	AG, CR, HR, LT, PT, UG, GM,	AL, CU, HU, LU, RO, UZ, KE,	AM, CZ, ID, LV, RU, VN, LS,	AT, DE, IL, MA, SD, YU, MW,	AU, DK, IN, MD, SE, ZA, MZ,	AZ, DM, IS, MG, SG, ZM, SD, GB,	BA, DZ, JP, MK, SI, ZW, SL,	EC, KE, MN, SK, AM, SZ,	EE, KG, MW, SL, AZ, TZ,	ES, KP, MX, TJ, BY, UG,	FI, KR, MZ, TM, KG, ZM,	GB, KZ, NO, TN, KZ, ZW,	GD, LC, NZ, TR, MD, AT,	GE, LK, OM, TT, RU, BE,	GH, LR, PH, TZ, TJ, CH,	TM
	TIC	2002	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
													20010316						
	US 2002183309			A1 20021203		US 2002-44493				21	1020.	33E TTT							
						CA 2002-2440238													
	EP 1370546						EP 2002-715079												
									FR,										
									MK,				•	·	•	•	•	•	
		2005						2005	0113		JP 2	002-	5737	67		20	0020	311	
PRAI		2001						2001	0316					•					
		2001						2001	0316										
		2002						2002											
		2002						2002											
0.0		2002				W		2002	0311										
os	OS MARPAT 137:247602																		

AB Title compds. I [wherein A = CO or covalent bond; D = O or S; L = alkylene, fluoroalkylene, or hydroxyalkylene; P and Q taken together form a covalent bond or are both H; R1 and R2 = independently H, (cyclo)alkyl, aryl(alkyl), cycloalkylalkyl, heterocyclyl(alkyl), hydroxyalkyl, alkenyl, or alkynyl; or NR1R2 = heterocyclyl; R3 = H, alkoxy(carbonyl), (halo)alkyl, alkylcarbonyl(oxy), alkylsufinyl, alkylsulfonyl, alkylthio, aryl, carboxy(alkyl), cyano(alkyl), formyl, halo(alkoxy), heterocyclyl, hydroxy(alkyl), SH, NO2, or (un)substituted amino(alkyl), carbamoyl, or sulfamoyl; R4-R7 = independently R3 or L2R20 or R20L3R22; L2 = alkylene, alkenylene, O, S, SO, SO2, CO, C:NOR21, or (un)substituted amino; L3 = covalent bond, alkylene, alkenylene, O, S, CO, N:OR21, or (un)substituted amino; R20 and R22 = independently aryl, heterocyclyl, or cycloalkyl; R21 = H or alkyl; or pharmaceutically acceptable salts, esters, amides, or prodrugs thereof] where prepared for modulation of the histamine-3 (H3) receptors. For example, 4-hydroxy-4'-cyanobiphenyl was treated with NaI, NaOH, and NaOCl in MeOH to give 4'-hydroxy-3'-iodo-[1,1'-biphenyl]-4carbonitrile (53%). Cyclization with 3-butyn-1-ol in DMF in the presence of CuI and Pd(PPh3)2Cl2 afforded 4-[2-(2-hydroxyethyl)-1-benzofuran-5yl]benzonitrile (95%). Mesylation (89%), followed by addition of (2R)-2-methylpyrrolidine•HBr and Na2CO3 in AcCN (34%), produced II. The latter displayed binding activity to H3 receptors in rat brain cortex tissue with Ki of 4.44 nM. I are H3 receptor ligands that modulate function of the H3 receptor by antagonizing its activity. Thus, I are useful for the treatment of disorders ameliorated by H3 receptor ligands, especially Alzheimer's disease, attention-deficit hyperactivity disorder, epilepsy, narcolepsy, obesity, cognitive impairment, deficits of memory, deficits of learning, and dementia (no data).

ΙI

IT 460748-54-3P, Ethyl 4'-hydroxy-3'-iodo-1,1'-biphenyl-3-carboxylate RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of (pyrrolidinylalkyl)benzofurans and analogs as histamine-3 receptor ligands for treatment of disorders related to CNS neurotransmission)

RN 460748-54-3 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 4'-hydroxy-3'-iodo-, ethyl ester (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:491850 CAPLUS

DN 115:91850

TI Optically active hydroxyarenecarboxylic acid 1-(trifluoromethyl)alkyl esters as intermediates for ferroelectric liquid crystals

IN Ozawa, Tetsuo; Fukahori, Choko

PA Mitsubishi Kasei Corp., Japan

SO Jpn. Kokai Tokkyo Koho, 7 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI JP 03058957	A2	19910314	JP 1989-195965	19890728	
PRAI JP 1989-195965		19890728			
00 100000 115 01050					

OS MARPAT 115:91850

GI

AB The title esters I [A = H; R = C2-18 alkyl, CH2CH2OR1, (CH2)3OR1, CH2CO2R1; R1 = C1-18 alkyl; X = lower alkyl, halo; n = 0, 1] (II) are prepared 3,4-Cl(AcO)C6H3CO2H (1.0 g) was treated with SOC12 under reflux for 3 h and the resulting acid chloride treated with 0.86 g (-)-Me(CH2)5CH(CF3)OH and triethylenediamine in toluene at 25° for 3 h to give 0.52 g I (A = Ac, R = hexyl, X = 3-Cl, n = 0), 0.5 g of which in (Me2CH)2O was treated with BuNH2 at room temperature for 12 h to give 0.45 g II (R = hexyl, X = 3-Cl, n = 0).

IT 135412-69-0P 135412-70-3P 135412-77-0P 135412-78-1P 135412-85-0P 135412-86-1P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for ferroelec. liquid crystals)

RN 135412-69-0 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 1-(trifluoromethyl)decyl ester (9CI) (CA INDEX NAME)

Ι

RN 135412-70-3 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 1-(trifluoromethyl)tridecyl ester (9CI) (CA INDEX NAME)

RN 135412-77-0 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 4-(heptyloxy)-1-(trifluoromethyl)butyl ester (9CI) (CA INDEX NAME)

RN 135412-78-1 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 3-(octyloxy)-1-(trifluoromethyl)propyl ester (9CI) (CA INDEX NAME)

RN 135412-85-0 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 3-(dodecyloxy)-3-oxo-1-(trifluoromethyl)propyl ester (9CI) (CA INDEX NAME)

RN 135412-86-1 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 3-butoxy-3-oxo-1-(trifluoromethyl)propyl ester (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:15021 CAPLUS

DN 114:15021

TI Optically-active 6-alkoxy-3-pyridinecarboxylic acid esters, liquid-crystal compositions containing them, and optical switching devices

IN Sugawara, Shungo

PA Nippon Telegraph and Telephone Corp., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp. CODEN: JKXXAF

DT Patent

LA Japanese .

FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI PRAI GI	JP 02056466 JP 1988-206385	A2	19900226 19880822	JP 1988-206385	19880822	

$$R^{1}O$$
 $CO_2$ 
 $L$ 
 $Y$ 
 $QR^2$ 

AB The title esters I (R1, R2 = C≥4 alkyl; L = CO2, OCO, direct bond; R1 and/or R2 = optically active; Q = CO2, O, direct bond; X, Y = H, halo; X and/or Y = halo; m =0, 1; L = direct bond and Q = CO2, O when m = 0), liquid-crystal compns. containing ≥1 I, and optical switching devices using I or liquid-crystal compns. containing ≥1 I are claimed. I or liquid-crystal compns. containing I have large spontaneous polarization and show

Ι

chiral smectic phase with wide mesomorphic range, thus permit quick response of display cell. 6-Decyloxynicotinic acid was treated with 3-fluoro-4-hydroxybenzoic acid, 1-methylheptyl 3-fluoro-4-hydroxybenzoate to give I [R1 = decyl, QR2 = CO2CHMe(CH2)5Me, L = CO2, m = 1; X = Y = 2-F] (II) showing a chiral smectic C phase. An optical switching cell packed with II was prepared

IT 128379-21-5P 130976-89-5P

RN 128379-21-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-bromo-4'-hydroxy-, 1-methylheptyl
ester (9CI) (CA INDEX NAME)

RN 130976-89-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 1-methylheptyl ester (9CI) (CA INDEX NAME)

L8 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:468511 CAPLUS

DN 113:68511

TI Optically-active biphenyl derivatives, liquid-crystal compositions, and optical switching devices

IN Sugawara, Shungo

PA Nippon Telegraph and Telephone Corp., Japan

SO Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡI	JP 02059544	A2	19900228	JP 1988-210541	19880826	
PRAI	JP 1988-210541		19880826			
OS	MARPAT 113:68511					

GI

$$\mathbb{R}^{1}\mathbb{Q}^{1}$$
 $\mathbb{R}^{2}$ 
 $\mathbb{Q}^{2}$ 
 $\mathbb{Q}^{3}\mathbb{R}^{2}$ 

AB The title derivs. I (R1, R2 = C≥4 alkyl; X1, X2 = F, C1; Y and/or Z = halo and the other = H; Q1 = O, OCO; Q2 = CO2, OCO; Q3 = CO2, O; R1 and/or R2 = optically-active), liquid-crystal compns. containing ≥1 I, and optical switching devices using I or liquid-crystal compns. containing ≥1 I are claimed. I or liquid-crystal compns. containing I show a chiral smectic C phase and permit quick response of display devices.

3-Fluoro-4-bromophenol was coupled with 3-fluoro-4-(1-methylheptyloxy)bromobenzene and the resulting biphenyl derivative was treated with 4-decyloxytetrafluorobenzoic acid to give I [Q1R1 = decyloxy, Q3R2 = optically-active OCHMe(CH2)5Me; Q2 = CO2, X1 = X2 = F, Y = 2-F, Z = 3-F] (II), showing a chiral smectic C phase. An optical switching cell packed

Ι

with II showed quick response.

IT 128379-19-1

RL: USES (Uses)

(Preparation and esterification with, of alkoxytetrahalobenzoic acids, chiral smectic C liquid crystals from)

RN 128379-19-1 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 2-methylbutyl ester (9CI) (CA INDEX NAME)

IT 128379-20-4 128379-21-5

RL: USES (Uses)

(condensation of, with pentahalobenzonitriles, in preparation of chiral smectic C liquid crystals)

RN 128379-20-4 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 1-methylheptyl ester (9CI) (CA INDEX NAME)

RN 128379-21-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-bromo-4'-hydroxy-, 1-methylheptyl ester (9CI) (CA INDEX NAME)

L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:85399 CAPLUS

DN 108:85399

TI Fluorobiphenyl benzoate derivative liquid crystals for optical switching devices for display

IN Shoji, Tadao; Osawa, Masashi; Takehara, Sadao; Fujisawa, Noburu; Ogawa, Hiroshi

PA Dainippon Ink and Chemicals, Inc., Japan; Kawamura Physical and Chemical Research Institute

SO Jpn. Kokai Tokkyo Koho, 7 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	JP 62181239	A2	19870808	JP 1986-22897	19860206	
	JP 07014899	B4	19950222			
PRAI GI	JP 1986-22897		19860206			

$$R \longrightarrow CO_2 \longrightarrow CO_2R^1$$

AB The title compds. I (R = C $\leq$ 20 alkyl, alkoxy; R1 = optically active group; X = H, halo) are useful for optical switching devices. The compds. show ferroelectricity and provide liquid-crystal display devices with rapid response. Thus, 4-C10H21OC6H4CO2H was refluxed with SOC12 and then treated with (S)-2-methylbutyl 3'-fluoro-4'-hydroxy-4-biphenylcarboxylate at 60-70° for 3 h and let stand overnight to give I [R = C10H21O, R1 = (S)-CH2CHMeEt, X = H] (II). A mixture of II 50 and (S)-2-methylbutyl 4-(3'-fluoro-4'-decyloxybiphenyl-4-carbonyloxy)benzoate (chiral smectic phase at 54.0-124.2°) 50% showed chiral smectic phase at 13.8-146.5° and response time 550  $\mu$ s at 65° when used in liquid crystal display cell.

IT 106316-31-8P

RL: PREP (Preparation)

(preparation and esterification of alkoxybenzoic acids with, in liquid-crystal

preparation)

RN 106316-31-8 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 2-methylbutyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- L8 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 1987:59023 CAPLUS
- DN 106:59023
- TI Liquid crystalline compounds having substituents
- IN Takehara, Sadao; Fujisawa, Toru; Arai, Yoshi; Kurokawa, Jitsuo
- PA Dainippon Ink Chemical Industry Co., Japan; Kawamura Physical and Chemical Research Institute
- SO Eur. Pat. Appl., 57 pp. CODEN: EPXXDW
- DT Patent

LA English FAN.CNT 2				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 188222	A2	19860723	EP 1986-100165	19860108
EP 188222	A3	19861105		
EP 188222	B1	19920429		
R: CH, DE, GB,	LI			
JP 61161244	A2	19860721	JP 1985-1791	19850109
JP 06029222	B4	19940420		
JP 61229841	A2	19861014	JP 1985-71628	19850404
JP 06029223	B4	19940420		
JP 61238762	A2	19861024	JP 1985-81688	19850417
JP 06029224	B4	19940420		
JP 61249953	A2	19861107	JP 1985-90676	19850426
JP 06078280	B4	19941005		
US 4828754	Α	19890509	US 1988-161421	19880223
PRAI JP 1985-1791	Α	19850109		
JP 1985-71628	Α	19850404	•	
JP 1985-81688	Α	19850417		
JP 1985-90676	Α	19850426		
US 1986-815935	A1	19860103		
OS CASREACT 106:59023	-			•
GI .				

$$R-Z-\left[\begin{array}{c} \\ \\ \end{array}\right]_{m}-CO_{2}-Z^{1}-\left[\begin{array}{c} \\ \\ \end{array}\right]_{n}-CO_{2}Q$$

AB Liquid crystal compds. for display devices are represented by I, where R is a C1-20 alkyl or alkoxy group; m and n are each 0 or 1, provided m and n are not 1 at the same time; Z is a 2-X-1,4-phenylene or 3-X-1,4-phenylene group and Z1 is a 2-Y-1,4-phenylene or 3-Y-1,4-phenylene group, where X and Y are each H, a halogen atom or a nitro group, provided X and Y are not H at the same time; and Q is an optically active group having a chiral C atom and a linear or cyclic alkyl or alkenyl group which may be substituted by a halogen atom. When Q is a 2-methylbutyl group, a 1-methylalkyl group having 4-8 C atoms, or a 2-chloropropyl group, the liquid crystal compound may have a chiral smectic C phase. Thus, 3-fluoro-4-dodecyloxybenzoic acid chloride 3.32 and (S)-2-methylbutyl 4'-hydroxybiphenyl-4-carboxylate 2.84 g were reacted in pyridine 10 and CH2Cl2 15 mL for 3 h under reflux. After the reaction mixture cooled, Et acetate 50 mL was added and washing twice with 10% HCl and once each with saturated NaHCO3 aqueous solution and saturated NaCl aqueous solution were performed. After the

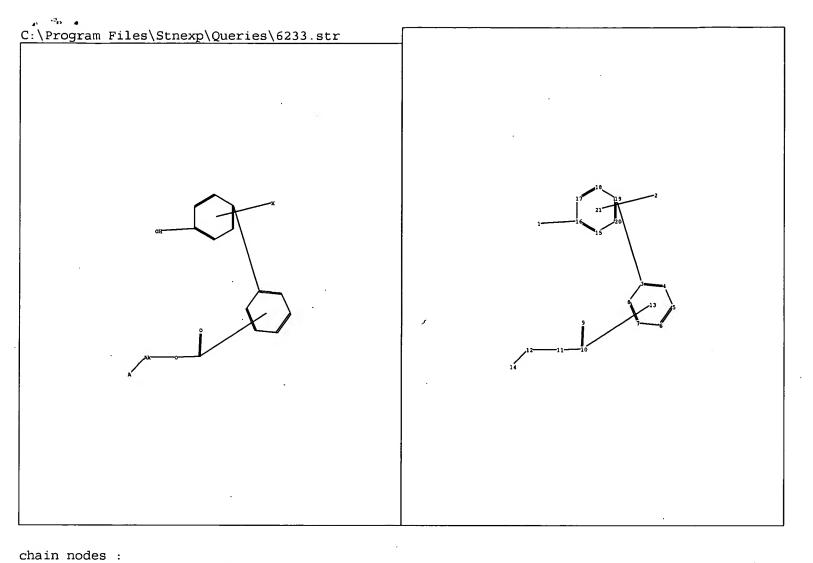
reaction. product was dried with anhydrous  ${\tt Na}$  sulfate, the solvent was concentrated

The crude crystals obtained were purified by column chromatog. on SiO2 gel with CHCl3/hexane and recrystd. from EtOH to obtain 4.64 g of 4-(4-[(S)-2-methylbutyloxycarbonyl]phenyl)phenyl 3-fluoro-4-dodecyloxybenzoate (II). II was heated at 160° to form an isotropic liquid and placed in a thin cell. The cell was cooled at 5°/min to align the smectic phase and a uniform monodomain was obtained. The cell was cooled to <118° to obtain a chiral smectic C phase. An elec. field (20 V, 50 Hz rectangular wave] was applied at 102° and the light switching action took 100  $\mu s$ . When a triangular wave was applied to the cell at 102° the spontaneous polarization was 2.24 nC/cm2.

IT 106316-31-8P

Absolute stereochemistry.

=>



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1 2 9 10 11 12 14

ring nodes:
    3 4 5 6 7 8 15 16 17 18 19 20

chain bonds:
    1-16 3-19 9-10 10-11 11-12 12-14

ring bonds:
    3-8 3-4 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds:
    1-16 9-10 10-11 11-12 12-14

exact bonds:
    3-19

normalized bonds:
    3-8 3-4 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
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Match level:
1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS